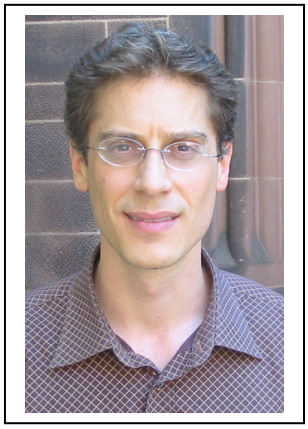

Victor S. Batista
Professor of Chemistry
Senior Editor – The Journal of Physical Chemistry

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Biography

Victor S. Batista was brought up in Buenos Aires, Argentina, and received his *Licenciado en Ciencias Quimicas* (B. Sc. in Chemistry) degree from the *Facultad de Ciencias Exactas y Naturales (FCEyN) de la Universidad de Buenos Aires* (University of Buenos Aires) in 1989.

In 1991 he moved to the United States and received his PhD degree in Chemistry from Boston University in 1996, where he also received the Sugata Ray Award in 1995 working under the mentorship of Prof. David F. Coker on the development of theoretical and computational methods to investigate photochemical reaction dynamics in the condensed phase. Following two postodoctoral research programs, working on semiclassical methods with Prof. William H. Miller at the University of California, Berkeley (1997–1999) and coherent-control techniques with Prof. Paul Brumer at the University of Toronto (2000-2001), he joined the Yale faculty as an Assistant Professor of Chemistry in 2001, where he became Associate Professor of Chemistry in 2005 and is now Professor of Chemistry since 2008. He was Director of Undergraduate Studies (2008-2010).

He has received the Innovation Award from Research Corporation (2002), the Hellman Family Junior Faculty Award from Yale University (2002); the Petroleum Research Funds Award G6 from the American Chemical Society (2002); the Career Award from the National Science Foundation (NSF) (2004); the Nanoscale Exploratory Research Award from NSF (2004); the Camille Dreyfus Teacher-Scholar Award (2005); an Alfred P. the Sloan Fellowship (2005–2006); co-chairmanship of the 2016 Vibrational Spectroscopy Gordon Conference; the 2016 Baker Lectureship at Cornell University; and the 2018 Harrison-MacRae Lectureship at Queen's University. He is a Visiting Scholar of Phi Beta Kappa for 2017-2018 . He is a member of the American Chemical Society (ACS PHYS Councillor 2018-Present), American Physical Society, and Biophysical Society.

His research interests include the development and application of semiclassical and quantum dynamics methods for studies of excited state reaction dynamics and

relaxation phenomena in polyatomic systems and semiconductor materials for solar-to-electric energy conversion and photocatalysis, as well as the development of quantum mechanics/molecular mechanics computational methods to study ligand binding interactions and reactivity in biomolecules, with emphasis on photoreceptors and water-splitting in photosystem II.

Current and Pending Support

Investigator: Batista, Victor

Support: Current
Project Title: Studies of Photosynthetic Reaction Centers and Biomimetic Systems
Source of Support: City University of New York
Total Project Award Amount: $265,000 Total Award Period Covered: 9/1/2018 - 8/31/2021
Location of Project: Yale University
Person Months Per Year Committed to the Project: Cal: Acad: Sum: 0.12

Support: Current
Project Title: Photocatalytic Assemblies for Solar Fuel Production
Source of Support: Department of Energy
Total Project Award Amount: $695,313 Total Award Period Covered: 3/1/2017 - 2/28/2020
Location of Project: Yale University
Person Months Per Year Committed to the Project: Cal: Acad: Sum: 0.10

Support: Current
Project Title: Argonne-Northwestern Solar Energy Research (ANSER) Center
Source of Support: Northwestern University/DOE
Total Project Award Amount: $1,696,290 Total Award Period Covered: 8/1/2014 - 1/31/2019
Location of Project: Yale University
Person Months Per Year Committed to the Project: Cal: Acad: Sum:

Support: Current
Project Title: Inverse Design, Development and Characterization of Catalytic Adsorbates at Semiconductor/Liquid Interfaces
Source of Support: Air Force Office of Scientific Research
Total Project Award Amount: $1,650,559 Total Award Period Covered: 4/15/2017 - 4/14/2020
Location of Project: Yale University
Person Months Per Year Committed to the Project: Cal: Acad: 0.50 Sum:

Support: Current
Project Title: Allosteric control of loop motions
Source of Support: National Science Foundation
Total Project Award Amount: $237,244 Total Award Period Covered: 8/1/2016 - 7/31/2020
Location of Project: Yale University
Person Months Per Year Committed to the Project: Cal: Acad: Sum: 0.25

Support: Current
Project Title: Collaborative Research: Bandgap Engineering of Dilute Antimonide III-Nitride Nanostructures for Efficient and Stable Photocatalytic Overall Water Splitting
Source of Support: National Science Foundation
Total Project Award Amount: $180,000 Total Award Period Covered: 5/1/2018 - 4/30/2021
Location of Project: Yale University
Person Months Per Year Committed to the Project: Cal: Acad: Sum: 0.25

Support: Current
Project Title: Computational and Biochemical Studies of Temperature Effects on Allostery in the Imidazole Glycerol Phosphate Synthase (IGPS) from T. maritima
Source of Support: National Institutes of Health/DHHS
Total Project Award Amount: $1,856,421 Total Award Period Covered: 9/1/2018 - 7/31/2022
Location of Project: Yale University
Person Months Per Year Committed to the Project: Cal: Acad: 1.00 Sum:

Support: Current
Project Title: Stretchable, Transparent & Biodegradable Electronic Material with Tunable Functionality
Source of Support: Defense Advanced Research Projects Agency (DARPA)
Total Project Award Amount: $509,699 Total Award Period Covered: 5/3/2018 – 11/2/2019
Location of Project: Yale University
Person Months Per Year Committed to the Project: Cal: Acad: Sum: 1.00

Support: Current
Project Title: Collaborative Research: Dinuclear Heterogeneous Catalysts (DHCs) as a New Platform for Selective Oxidation of CO and Methane
Source of Support: National Science Foundation
Total Project Award Amount: $180,000 Total Award Period Covered: 8/15/2018 - 7/31/2021
Location of Project: Yale University
Person Months Per Year Committed to the Project: Cal: Acad: Sum: 0.25

Support: Pending
Project Title: Mining Air for Fuels and Fine chemicals
Source of Support: Arizona State University/DOE
Total Project Award Amount: $1,666,825 Total Award Period Covered: 2/1/2019 - 1/31/2022
Location of Project: Yale University
Person Months Per Year Committed to the Project: Cal: Acad: 0.25 Sum: 0.50

Support: Pending
Project Title: CCI Phase I: NSF Center for Strong Coupling of Nanomaterials to Nanomaterials and Organic Moieties (Pre-proposal)
Source of Support: National Science Foundation
Total Project Award Amount: $1,800,000 Total Award Period Covered: 9/1/2019 - 8/31/2022
Location of Project: Yale University
Person Months Per Year Committed to the Project: Cal: Acad: Sum:

Support: Pending
Project Title: Collaborative Research: Dinuclear Heterogeneous Catalysts (DHCs) as a New Platform for Selective Oxidation of CO and Methane (This proposal)
Source of Support: National Science Foundation
Total Project Award Amount: $200,000 Total Award Period Covered: 6/1/2019 - 7/31/2022
Location of Project: Yale University
Person Months Per Year Committed to the Project: Cal: Acad: Sum: 0.12

Professional Preparation

Universidad de Buenos Aires (UBA): B.Sc. in Chemistry, 1989
Boston University: Theoretical Chemistry Ph.D. 1997
University of California, Berkeley: Theoretical Chem. Post-Doc. 1999
University of Toronto: Theoretical Chem. Post-Doc 2001

Appointments

July 2008-present: Professor, Department of Chemistry, Yale University
April 2011-present: Senior Editor, Journal of Physical Chemistry.
July 2008-July 2010: Director of Undergraduate Studies, Department of Chemistry, Yale University
July 2005-2008: Associate Professor of Chemistry, Department of Chemistry, Yale University.
March 2001-July 2005: Assistant Professor of Chemistry, Department of Chemistry, Yale University.

Selected Honors, Awards and Professional Service
2002 ACS PRF-G6 Award
2002 Hellman Family Junior Faculty Award
2002 Research Corporation Innovation Award
2004 NSF Career Award
2004 NSF Nanoscale Exploratory Research Award
2005-2006 Alfred P. Sloan Fellow
2005 Camille Dreyfus Teacher-Scholar Award
2005-2006 Yale Junior Faculty Fellow in the Natural Sciences
2016 Co-chairman of the Vibrational Spectroscopy Gordon Conference
2016 Baker Lecture, Cornell Univeristy
2017-2018 Phi Beta Kappa Visiting Scholar
2018 Harrison-MacRae Lecture, Queen's University
2018- ACS PHYS Councillor
Member: American Chemical Society, Biophysical Society

Synergistic Activities
Referee of scientific journals: Nature, Science, Proteins, Annual Review of Physical Chemistry, Proceedings of the National Academy of Science (U.S.A), Biophysical Journal, Journal of Chemical Physics, Chemical Physics Letters, Journal of Physical Chemistry, Journal of Inorganic Biochemistry, Journal of Chemical Theory and Computation, Journal of Computational and Theoretical Chemistry.

Panel reviewer committee member:
2013-2017 NIH MSFA Permanent Member; 2015 NSF CCI Panelist; 2015 DOE PNNL Panelist; 2014-2013 DOE JCAP Review Panelist; 2013; DOE Career Program; 2013 NIH MSFE Study Section; 2013 NSF CHE Committee of Visitors; 2013 NSF CHE Theory Panel; 2012 NSF CCI Panel; 2012 NIH MSFE Study Section; 2012 DOE Career Panel; DOE Theoretical Chemistry Review Panel, 2011; DOE BES Committee of Visitors,

2011; Chair, European Science Foundation Review Panel, EuroSolar Energy Program 2010; DOE Theoretical Chemistry Review Panel, 2009;NSF Review Panel Career Program, 2009; NSF Review Panel Collaborative Research in Chemistry, 2005; Member, NSF Review Panel Career Program, 2005; Member, NSF Review Panel MRI in Chemistry, 2004.

Teacher mentor for the K-12 educational program e-mentoring initiative: Society for Advancement of Chicanos and Native Americans in Science (SACNAS).

Faculty service committees:
Graduate Admissions
Theory Faculty Search Committee
Junior Faculty Mentoring Committees
Planning Committee

Teaching:
Spring 2017 CHEM 430/530, Statistical Mechanics and Thermodynamics
Fall 2017 CHEM 470/570, Quantum Mechanics
Fall 2017 CHEM 505, Alternative Energy

Undergraduate research mentor: Underrepresented minority students enrolled in the STARS program at Yale University.

Developer of pedagogical web sites
http://ursula.chem.yale.edu/~batista/classes/vaa/index.html
http://ursula.chem.yale.edu/~batista/classes/v572/index.html
http://ursula.chem.yale.edu/~batista/classes/CHEM505/index.html
http://ursula.chem.yale.edu/~batista/classes/vvv/index.html
http://ursula.chem.yale.edu/~batista/classes/114/index.html
http://ursula.chem.yale.edu/~batista/classes/tutorials/index.html
http://wikidchem.org

Identification of Potential Conflicts of Interest
Sr. Collaborators, Co-authors and Co-editors During the Past Four Years and Current Affiliations
Allen, Laura, The Scotts Miracle-Gro Company; **Altavilla, Salvatore**, University of Bologna; **Amin, Muhamed**, Lawrence Berkeley National Lab; **Anfuso, Chantelle**, Georgia Gwinett College; **Angeles-Boza, Alfredo**, M. University of Connecticut; **Batista, Enrique,** Los Alamos Nat. Lab.; **Batra, Arunabh**, Columbia University; **Benedict, Jason**, SUNY Buffalo; **Bisquert, Juan**, Jaume I University of Castello; **Block, Eric**, SUNY Albany; Bocarsly, Andrew, Princeton; **Bonvicini, Andreas**, University of Bologna; **Brennan, Bradley**, California Inst. of Techn.; **Brewster, Timothy**, Memphis; **Robert, Bruno**, CNRS; Buda, Francesco, Leiden University; Campos, Jesus, University of Oxford; **Chabolla, Steven**, UC Irvine; **Chen, Lin,** Northwestern University; **Chen, Xin**, Xi'an Jiaotong University; **Chernev, Petko**, Free University of Berlin; **Chidsey, Christopher**, Stanford University; **Coronado, Eugenio,** University of Zaragoza;

Demoulin, Jean-Baptiste, University in Ottignies-Louvain-la-Neuve; **Dethier, Berenice**, SUNY Albany; **Dobbins, Tabbetha**, Rowan University; **Doerrer, Linda**, Boston University; **El-Tahawy, MMT**, Damanhour University; **Est, Art, van der**, Brock University; **Fichtl,, Christopher**, Los Alamos Nat. Lab.; **Francas, Laia**, Imperial College London; **Garavelli, Marco**, University of Bologna; **Gascon Jose**,; **Ge, Aimin**, Emory University; **Geiger, Franz**, Northwestern University; **Grabowski, Paul**, UC Irvine; **Graziani, Frank**, Vanderbilt; **Grice, Kyle**, A. DePaul University; **Groot, Huub,** De Leiden University; **Gundala, Sivaji,** SUNY Albany; **Gunner, Marilyn**, CUNY City College; **Guo, Ying**, Georgia Gwinnett; **Gust, Devens**, ASU; **Han Du, Wen-Ge** Scripps at La Jolla; **Haumann, Michale**, Free University of Berlin; **Hildebrandt, Peter**, Technical University of Berlin; **Hong, Jiyun,** Northwestern; **Hopkins, Michael**, University of Chicago; **Huppert, Dan**, Tel Aviv Univ.; **Hybertsen, Mark**, Brookhaven Nat. Lab**.; Jang, Seogjoo**, CUNY Queens College; **Jarzembska, Katarzyna**, University of Warsaw; **Jia, Yanyan**, Emory University; **Jia, Yaoyao,** Korea University; **Jiang, Huihong,** Shanghai Jiaotong University School of Medicine,; **Khan, Sahr,** MIT; **Kharche, Neerav,** Brookhaven Nat. Lab.; **Kim, Yeonji**, Korea University; **Koenigsmann, Christopher**, Fordham University; **Koepf, Matthieu**, Alternative Energies and Atomic Energy Commission (France); **Koeppe, Benjamin,** Humboldt University of Berlin; **Kubiak, Clifford**, UCSD; **Kwon, Gihan,** Argonne Nat. Lab.; **Lakkaraju, Prasad**, Georgian Court University; Lee, Ji, Hae Korea University; Lee, Sung-Joon, Korea University; **Lee, Sung-Joon**, Korea University; **Leszczynski, Jerzy**, Jackson State University; **Li, Gonghu,** University of New Hampshire; Li, **Shengju, Shanghai** Jiaotong University School of Medicine,; **Li, Zhen**, Shanghai Jiaotong University School of Medicine,; **Lian, Tianquan**, Emory University; **Liu, Jian**, Newport Corporation; **Llobet, Antoni**, ICIQ (Spain); Lu, Zhou, Chinese Academy of Sciences; **Machan, Charles**, University of Virginia; **Mara, Michael**, Argonne Nat. Lab.; **Matheu, Roc**, ICIQ (Spain); **Matsunami, Hiroaki,** Duke University; **McNamara, William**, College of William, and Mary; **Mifflin, Amanda**, University of Puget Sound; Milot, Rebecca, University of Oxford; **Miller, William**, University of California, Berkeley; **Mooney, Victoria**, National High Magnetic Field Laboratory; **Moore, Ana**, ASU; **Moore, Thomas**, ASU; **Muckerman, James**, Brookhaven Nat. Lab.; **Nenov, Artur**, University of Bologna; **Nibbering, Erik**, Max Born Institute; **Noodelman, Louis**, Scripps; **Oviedo, M**., Belen University of California, Riverside; **Pan, Yi,** Nanjing University; Pander, James, Princeton; **Petersen, Poul,** Cornell; **Pines, Dina**, Ben Gurion University; **Pines, Ehud**, Ben Gurion University; **Piotrowiak, Piotr,** Rutgers University; **Poddutoori, Prashanth,** Brock University; **Poluektov, Oleg, G.** Argonne; **Ragain, Christina**, Southeast Missouri State University; **Rego, Luis**, University of Florianopolis; **Ricci, Clarisse,** UCSD; **Richards, David**, Lawrence Livermore National Lab; **Ripolles, Teres**a, Kyushu Institute of Technology; **Ryan, Kevin**, CUNY City College; Sala, Xavier, UAB (Barcelona); **Sánchez, Cristián**, National University of Cordoba; **Santos, Lea, F.** Yeshiva University; Segarra-Martí, Javier, University of Bologna; **Sheehan, Stafford,** Catalytic Innovations; **Silveira, Rodrigo,** University of Campinas; Skaf, Munir, University of Campinas; **Soloveichik, Grigorii**, GE Global Research; Song, Hee-eun, Korea Institute of Energy Research; **Song, Jia**, Emory University; **Tanski, Joseph**, Vassar College; **Thomson, Regan,** Northwestern University; **Tiede, David**, Argonne Nat. Lab.; **Torre, Jose**, Jaume I University of Castello; **Velarde, Luis**, SUNY Buffalo;

Venkataraman,, Latha Columbia University; **Venkatesan, T., Venky** NUS; **Vinyard, David**, Louisiana State University; **Waldie, Kate,** UCSD; **Wang, Hong-Fei**, PNNL; **Wasielewski, Michael**, Northwestern University; **Waymouth, Robert**, Stanford University; **Wu, Chunyan**, Korea University; **Xie, Zhao-Xiong**, Xiamen University; **Yan, Yong**, Princeton; **Young, Karin**, Centre College;

Graduate and Postdoctoral Advisors

Ph.D. Advisor: **Prof. David Coker**, Boston University, Dept. of Chemistry
Postdoc Advisor: **Prof. Kenneth Sauer**, Univ. of California, Berkeley, Dept. of Chemistry
Postdoc Advisor: **Prof. Paul Brumer**, Univ. of Toronto, Dept. of Chemistry

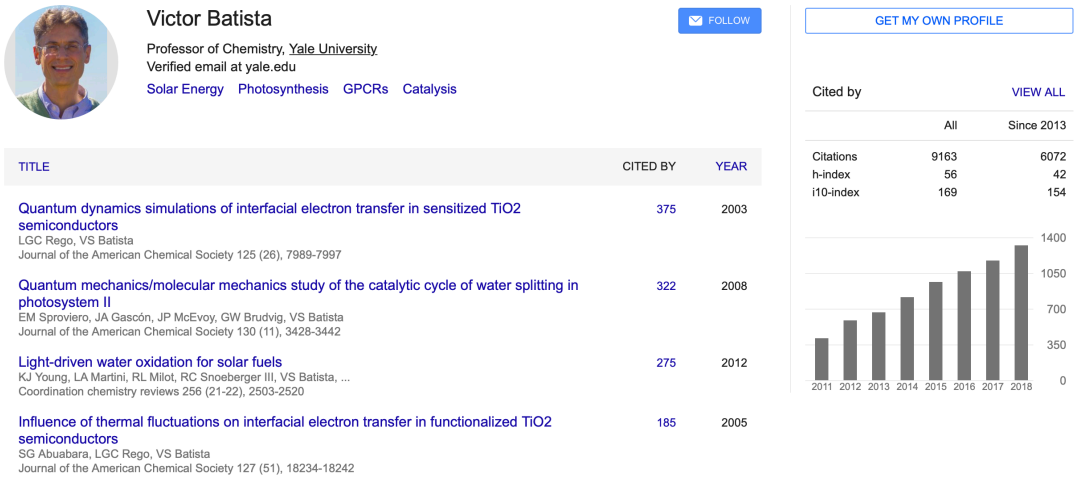
Graduate Students and Postdoctoral Associates

(total number of Ph.D. students supervised = 16; total number of postdoctoral associates supervised = 31)

Abuabara, Sabas, HBK NY LLC**, Askerka, Mikhail**, University of Toronto; **Chen, Xin**, Xian Jiantong University; **Flores, Samuel**, Uppsala University; **Freeze, Jessica**, Yale; **Greene, Samuel**, Yale; **Kelly, Harvey**, Yale; **Chaudhuri, Subhajyoti**, Yale; **Ding, Wendu**, Northwestern University; **Kong, Xiangmeng**, Yale; **Jung, Kenneth**, Yale; **Matula, Adam**, Yale; **Newcomer, Michael**, The D.E. Shaw Group; **Reiss, Krystle**, Yale; **Rudshteyn, Benjamin**, Yale; **Snoeberger, Ning-Shiuan**, MIT; **Snoeberger III, Robert**, Google; **Wu, Yinghua**, Elmagin Capital.

Acharya, Atanu, Yale; **Ahmed, Lucky**, Yale; **Araujo, Carlos**, Uppsala University; **Ertem, Mehmed**, Brookhaven Nat. Lab.; **Fernando, Amendra**, MIT; **Banerjee, Sandipan,** Intel; **Gascon, Jose**, University of Connecticut; **Hedstrom, Svante**, Stockholm University**; Hendrickson, Heidi**, Lafayette College; **Hermann, Carmen**, University of Hamburg; **Ho, Junming**, University of New South Wales; **Konezny, Steven**, Yale, Energy Sciences Institute; **Luber, Sandra**, University of Zurich; **Markmann, Andreas**, Capital One; **Morzan, Uriel**, Yale; **Mendez-Hernandez, Dalvin**, University of Puerto-Rico, Cayey; **Negre, Christian**, Los Alamos Nat. Lab.; **Ozbil, Mehmet**, Istanbul Arel University; **Pal, Rhitankar**, Intel; **Palma, Julio**, Penn State Fayette; **Psciuk, Brian**, Argus; **Rego, Luis**, Federal University of Santa Cantarina, Brazi; **Rivalta, Ivan**, Laboratoire de Chimie Ens de Lyon; **Sekharan, Sivakumar**, CCDC, Rutgers; **Sproviero, Eduardo**, University of the Sciences; **Videla, Pablo**, Yale; **Vogt, Leslie**, NYU; **Warnke, Ingolf**, Halo Tech Software; **Wang, Ting**, N/A; **Xiao, Dequan**, University of New Haven; **Yang, Ke**, Yale.

Impact Factor (h=56, Google Scholar, Citations=9163)



Publications (total 258):

1. Batista, V. S.; Coker, D. F. Nonadiabatic Molecular Dynamics Simulation of Photodissociation and Geminate Recombination of I2 Liquid Xenon. J. Chem. Phys. 1996, 105 (10), 4033-4054.
2. Batista, V. S.; Coker, D. F. Nonadiabatic Molecular Dynamics Simulation of Ultrafast Pump-Probe Experiments on I2 in Solid Rare Gases. J. Chem. Phys. 1997, 106 (17), 6923-6941.
3. Batista, V. S.; Coker, D. F. Nonadiabatic Molecular Dynamics Simulations of the Photofragmentation and Geminate Recombination Dynamics in Size-Selected I2-Arn Cluster Ions. J. Chem. Phys. 1997, 106 (17), 7102-7116.
4. Batista, V. S.; Miller, W. H. Semiclassical Molecular Dynamics Simulations of Ultrafast Photodissociation Dynamics Associated With the Chappuis Band of Ozone. J. Chem. Phys. 1998, 108 (2), 498-510.
5. Batista, V. S.; Coker, D. F. On Nonadiabatic Molecular Dynamics Simulations of the Photofragmentation and Geminate Recombination Dynamics in Size-Selected I2-Arn Cluster Ions (vol 106, pg 7102, 1997). J. Chem. Phys. 1999, 110 (13), 6583-6584.
6. Batista, V. S.; Zanni, M. T.; Greenblatt, B. J.; Neumark, D. M.; Miller, W. H. Femtosecond Photoelectron Spectroscopy of the I2- Anion: A Semiclassical Molecular Dynamics Simulation Method. J. Chem. Phys. 1999, 110 (8), 3736-3747.
7. Guallar, V.; Batista, V. S.; Miller, W. H. Semiclassical Molecular Dynamics Simulations of Excited State Double-Proton Transfer in 7-Azaindole Dimers. J. Chem. Phys. 1999, 110 (20), 9922-9936.
8. Zanni, M. T.; Batista, V. S.; Greenblatt, B. J.; Miller, W. H.; Neumark, D. M. Femtosecond Photoelectron Spectroscopy of the I2- Anion: Characterization of the (Ã′2Πg,1/2 Excited State. J. Chem. Phys. 1999, 110 (8), 3748-3755.
9. Coronado, E. A.; Batista, V. S.; Miller, W. H. Nonadiabatic Photodissociation Dynamics of ICN in the Ã Continuum: A Semiclassical Initial Value Representation Study. J. Chem. Phys. 2000, 112 (13), 5566-5575.
10. Guallar, V.; Batista, V. S.; Miller, W. H. Semiclassical Molecular Dynamics Simulations of Intramolecular Proton Transfer in Photoexcited 2-(2 '-Hydroxyphenyl)-

Oxazole. J. Chem. Phys. 2000, 113 (21), 9510-9522.
11. Batista, V. S.; Brumer, P. Semiclassical Dynamics in the Coherent Control of Nonadiabatic ICN Photodissociation. J. Phys. Chem. A 2001, 105 (12), 2591-2598.
12. Batista, V. S.; Brumer, P. A Direct Approach to One Photon Interference Contributions in the Coherent Control of Photodissociation. J. Chem. Phys. 2001, 114 (23), 10321-10331.
13. Batista, V. S.; Brumer, P. On Coherent Control in the Presence of Intrinsic Decoherence: Proton Transfer in Large Molecular Systems (vol 89, art no 143201, 2002). Phys. Rev. Lett. 2002, 89 (24), 249903.
14. Batista, V. S.; Brumer, P. Coherent Control in the Presence of Intrinsic Decoherence: Proton Transfer in Large Molecular Systems. Phys. Rev. Lett. 2002, 89 (14), 143201.
15. Burant, J. C.; Batista, V. S. Real Time Path Integrals Using the Herman-Kluk Propagator. J. Chem. Phys. 2002, 116 (7), 2748-2756.
16. Guallar, V.; Harris, D. L.; Batista, V. S.; Miller, W. H. Proton-Transfer Dynamics in the Activation of Cytochrome P450eryF. J. Am. Chem. Soc. 2002, 124 (7), 1430-1437.
17. Wu, Y.; Batista, V. S. Semiclassical Molecular Dynamics Simulations of the Excited State Photodissociation Dynamics of H2O in the A 1B1 band. J. Phys. Chem. B 2002, 106, 8271-8277.
18. Batista, V. S.; Brumer, P. In Coherent Control: Principles and Semiclassical Implementations, Quantum Control: Mathematical and Numerical Challenges, Bandrauk, A. D.; Delfour, M. C.; Bris, C. L., Eds. 2003; pp 59-78.
19. Rego, L. G. C.; Batista, V. S. Quantum Dynamics Simulations of the Interfacial Electron Transfer in Sensitized TiO2 Semiconductors. J. Am. Chem. Soc. 2003, 125, 7989-7997.
20. Wu, Y.; Batista, V. S. Erratum: “Matching-Pursuit for Simulations of Quantum Processes” [J. Chem. Phys. 118, 6720 (2003)]. J. Chem. Phys. 2003, 119 (14), 7606-7606.
21. Wu, Y. H.; Batista, V. S. On Matching-Pursuit for Simulations of Quantum Processes (vol 118, pg 6720, 2003). J. Chem. Phys. 2003, 119 (14), 7606-7606.
22. Wu, Y. H.; Batista, V. S. Matching-Pursuit for Simulations of Quantum Processes. J. Chem. Phys. 2003, 118 (15), 6720-6724.
23. Flores, S. C.; Batista, V. S. Model Study of Coherent-Control of the Femtosecond Primary Event of Vision. J. Phys. Chem. B 2004, 108 (21), 6745-6749.
24. Gascon, J. A.; Batista, V. S. QM/MM Study of Energy Storage and Molecular Rearrangements Due to the Primary Event in Vision. Biophys. J. 2004, 87 (5), 2931-2941.
25. Wu, Y. H.; Batista, V. S. Quantum Tunneling Dynamics in Multidimensional Systems: A Matching-Pursuit Description. J. Chem. Phys. 2004, 121 (4), 1676-1680.
26. Abuabara, S. G.; Rego, L. G. C.; Batista, V. S. Influence of Thermal Fluctuations on Interfacial Electron Transfer in Functionalized TiO2 Semiconductors. J. Am. Chem. Soc. 2005, 127 (51), 18234-18242.
27. Chen, X.; Wu, Y. H.; Batista, V. S. Matching-Pursuit/Split-Operator-Fourier-Transform Computations of Thermal Correlation Functions. J. Chem. Phys. 2005, 122 (6).
28. Gascon, J. A.; Sproviero, E. M.; Batista, V. S. QM/MM Study of the NMR

Spectroscopy of the Retinyl Chromophore in Visual Rhodopsin. J. Chem. Theor. Comp. 2005, 1 (4), 674-685.
29. McEvoy, J. P.; Gascon, J. A.; Batista, V. S.; Brudvig, G. W. The Mechanism of Photosynthetic Water Splitting. Photochem. Photobiol. 2005, 4, 940-949.
30. McEvoy, J. P.; Gascon, J. A.; Sproviero, E. M.; Batista, V. S.; G.W., B. Computational Structural Model of the Oxygen Evolving Complex in Photosystem II: Complete Ligation by Protein, Water and Chloride. In Photosynthesis: Fundamental Aspects to Global Perspectives, Bruce, D.; van der Est, A., Eds. Allen Press, Inc.: Lawrence, Kansas, 2005; Vol. 1, pp 278-280.
31. Rego, L. G. C.; Abuabara, S. G.; Batista, V. S. Model Study of Coherent Quantum Dynamics of Hole States in Functionalized Semiconductor Nanostructures. J. Chem. Phys. 2005, 122 (15), 154709.
32. Rego, L. G. C.; Abuabara, S. G.; Batista, V. S. Coherent Optical Control of Electronic Excitations in Functionalized Semiconductor Nanostructures. Quant. Inform. Comput. 2005, 5 (4-5), 318-334.
33. Wu, Y. H.; Herman, M. F.; Batista, V. S. Matching-Pursuit/Split-Operator Fourier-Transform Simulations of Nonadiabatic Quantum Dynamics. J. Chem. Phys. 2005, 122 (11).
34. Abuabara, S. G.; Gascon, J. A.; Leung, S. Y.; Batista, V. S. Force Field Parameters for Large-Scale Computational Modeling of Sensitized TiO2 Surfaces. Proc. SPIE 2006, 6325, 6325R 1-12.
35. Chen, X.; Batista, V. S. Matching-Pursuit/Split-Operator-Fourier-Transform Simulations of Excited-State Nonadiabatic Quantum Dynamics in Pyrazine. J. Chem. Phys. 2006, 125 (12).
36. Gascon, J. A.; Leung, S. S. F.; Batista, E. R.; Batista, V. S. A Self-Consistent Space-Domain Decomposition Method for QM/MM Computations of Protein Electrostatic Potentials. J. Chem. Theor. Comp. 2006, 2 (1), 175-186.
37. Gascon, J. A.; Sproviero, E. M.; Batista, V. S. Computational Studies of the Primary Phototransduction Event in Visual Rhodopsin. Acc. Chem. Res. 2006, 39 (3), 184-193.
38. Leung, K.; Rempe, S. B.; Schultz, P. A.; Sproviero, E. M.; Batista, V. S.; Chandross, M. E.; Medforth, C. J. Density Functional Theory and DFT+U Study of Transition Metal Porphines Adsorbed on Au(111) Surfaces and Effects of Applied Electric Fields. J. Am. Chem. Soc. 2006, 128 (11), 3659-3668.
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Research Accomplishments

Time-Dependent Methods: The Batista group has developed time-dependent methods for simulations of quantum reaction dynamics in polyatomic systems, including algorithms based on time-sliced semiclassical and full quantum-mechanical propagators (*e.g.*, the MP/SOFT method). Applications of these methods were focused on ultrafast relaxation processes that produce broad and structureless absorption spectra of polyatomic systems, including nonadiabatic dynamics, excited state intramolecular proton transfer, and photoinduced isomerization processes in excited electronic states. These studies found that the spectral consequence of ultrafast relaxation processes is to mask the structural and dynamical information necessary to describe chemical reactivity at the molecular level, and that computational modeling is essential to provide insight into the nature of reaction dynamics and rigorous assignments of spectroscopic measurements.

Thermal Correlation Functions: In addition to quantum dynamics studies based on propagation of multidimensional wavefunctions, the Batista group has generalized the MP/SOFT algorithm to evaluate thermal-equilibrium density matrices, thermal correlation functions, and finite-temperature time-dependent expectation values. The generalized MP/SOFT method exploits the analogy between the time-dependent Schrödinger equation and the Bloch equation and computes finite-temperature density matrices via imaginary-time propagation, avoiding the "sign problem" that usually defies the capabilities of real-time path-integral Monte Carlo. The Heisenberg time-evolution operators, involved in thermal correlation functions, are analogously computed by real-time propagation.

Electronic Relaxation in Sensitized Semiconductors: Computational studies of sensitized semiconductor surfaces by the Batista group focused on TiO_2 anatase surfaces functionalized with organic and inorganic molecules, including molecular linkers commonly used in Grätzel cells. The studies characterized the nature of interfacial electron transfer mechanisms that for many years have challenged conventional electron transfer theories formulated in the weak-coupling limit. The studies addressed the dynamics of photoinduced electron-hole pair relaxation at the molecular level, and the subsequent carrier diffusion mechanism after electron injection in the conduction band. In addition, coherent control scenarios based on sequences of ultrafast unitary laser pulses were computationally demonstrated, predicting the feasibility of creating and manipulating coherent electronic excitations on monolayers of adsorbate molecules covalently attached to TiO_2 semiconductor surfaces.

Force Field Parameters: Force field parameters for large-scale computational modeling of sensitized TiO_2 surfaces have been developed from the energetic analysis of minimum energy configurations and ensembles of thermal configurations generated by DFT molecular dynamics simulations. The resulting force field, composed of Coulomb, van der Waals and harmonic interactions is an extension of Amber and reproduces *ab initio* minimum energy structures and phonon spectra density profiles of sensitized TiO_2-anatase nanostructures. Furthermore, simulations of interfacial electron injection and electron-hole relaxation dynamics have demonstrated the capabilities of the resulting molecular mechanics force field parameters for accurate modeling nuclear fluctuations responsible for speeding up the interfacial electron transfer dynamics in sensitized

semiconductor surfaces at finite temperature. The resulting force field thus offers an opportunity to study models beyond the capabilities of DFT molecular dynamics methods, including adsorbate molecules covalently attached to semiconductor surfaces in complex molecular environments (liquids).

Photocatalysis: Computational studies of TiO_2 surfaces sensitized with oxomanganese surfaces by the Batista group predicted visible-light sensitization based on TiO_2 surface functionalization with oxomanganese complexes. The simulations also suggested the possibility of visible-light photoactivation of Mn catalysts attached to semiconductor surfaces. These results motivated Batista to initiate a collaboration with 3 experimental groups at Yale (including Brudvig, Crabtree and Schmuttenmaer) in a joint experimental and theoretical effort to investigate TiO_2 functionalization for solar-light water-splitting and other applications of green-oxidation chemistry in the absence of primary oxidants. The team has already demonstrated, in practice, the feasibility of sensitizing TiO_2 to absorption of visible light by surface functionalization with Mn-catalysts, and the possibility of activating Mn(III) catalysts by ultrafast interfacial electron injection.

Water Splitting in Photosystem II: The DFT-QM/MM studies of photosystem II (PSII) by Batista and coworkers addressed the development of chemically sensible models of the oxygen-evolving complex (OEC) in the $S_0 \rightarrow S_4$ states. The OEC of PSII is a paradigm system for engineering direct solar fuel production systems since it involves a catalyst with inexpensive and abundant metals (calcium and manganese) and is capable of splitting water by accumulating sufficient oxidizing power. The resulting scientific insight on structure/function relations provided by these computational studies of PSII has been useful not only to understand fundamental chemistry of oxygen evolution by natural photosynthesis, but also for studies of water splitting by artificial photosynthetic systems, including TiO_2 sacrificial electron-acceptor surfaces functionalized with oxomanganese catalysts.

Studies of Visual Rhodopsin: Computational studies of visual rhodopsin by Batista and coworkers have addressed the molecular rearrangements induced by the primary photochemical event responsible for phototransduction and energy storage. These studies provided fundamental insight on long-standing problems regarding the assembly and function of the individual amino acid residues and bound water molecules at the active site of this prototypical G-protein coupled receptor (GPCR) that is responsible for triggering the signal transmission cascade in vertebrate vision.

Coherent Control: The Batista group has developed quantum control scenarios for laser manipulation of electronic excitations in sensitized semiconductor surfaces. Building on earlier work on coherent-control of reaction dynamics in excited electronic states, it was found that superexchange hole tunneling through adsorbate molecules can be inhibited and eventually halted by applying sufficiently frequent unitary pulses that exchange energy with the system but do not collapse the coherent evolution, or affect the underlying electron transfer energy barriers.

Presentations (last 5 years, in reverse chronological, >283 total)

1. **August 20, 2018:** Symposium LightChEC 2018 - University of Zurich, Zurich, Switzerland.
2. **August 19-23, 2018:** "Fundamental Understandings of Catalysis at Interfaces" Symposium at the 255th ACS National Meeting, Boston, MA, USA..
3. **July 22-July 27, 2018:** 2018 Gordon Conference on Computational Chemistry - Mount Snow, West Dover, Vermont.
4. **July 17-July 21, 2018:** 2018 Condensed Phase Dynamics Workshop - Telluride, Colorado.
5. **July 11-July 13, 2018:** CECAM Workshop: Frontiers and challenges of computing metals for biochemical, medical and technological applications" - Paris, France.
6. **June 24-June 27, 2018:** Photoinduced processes in Embedded Systems - University of Pisa, Pisa, Italy.
7. **June 19-June 21, 2018:** NSF KI-Net Mathematical and Numerical Aspects of Quantum Dynamics Workshop - University of Maryland, College Park, Maryland.
8. **June 8-June 11, 2018:** Molecular Sciences Software Institute Workshop: Modular Software Infrastructure for Excited State Dynamics - University of Buffalo, Buffalo, New York.
9. **June 4-7, 2018: 40th** DOE Solar Photochemistry Principal Investigators Meeting, Gaithersburg, Maryland.
10. **May 22-May 24, 2018:** 2018 AFOSR Molecular Dynamics/Theoretical Chemistry Program Review, Philips Technology Institute (PTi) on Kirtland Air Force Base, Albuquerque, NM.
11. **Apr 5-Apr 6, 2018:** Phi Beta Kappa Visiting Scholar Visit - University of Notre Dame, Notre Dame, IN, USA.
12. **Mar 19-Mar 23, 2018:** Photosynthesis/Bioenergetics Workshop on Oxygen Evolution and Reduction, Institute of Advanced Studies, Nanyang Technological University, Singapore.
13. **Mar 18-Mar 22, 2018:** "Computational Catalyst Design for Energy Conversion and Storage" Symposium at the 255th ACS National Meeting, New Orleans, LA, USA.
14. **Mar 15-Mar 16, 2018:** Phi Beta Kappa Visiting Scholar Visit - Louisiana State University, Baton Rouge, LA, USA**.**
15. **Mar 7, 2018:** ANSER Principal Investigators Workshop - Northwestern University, Evanston, IL, USA.
16. **Mar 2-Mar 5, 2018:** 3rd Molecules and Materials for Artificial Photosynthesis Conference, Cancun, Mexico.
17. **Feb 15-Feb 16, 2018:** Phi Beta Kappa Visiting Scholar Visit - Auburn University, Auburn, AL, USA.
18. **Feb 12-Feb 13, 2018:** Phi Beta Kappa Visiting Scholar Visit - University of Alabama, Tuscaloosa, AL, USA.
19. **Feb 9, 2018:** Harrison / MacRae Lecture Series - Department of Chemistry and Physics - Queen's University, Kingston, ON, Canada.

20. **Jan 28-Feb 2, 2018:** Renewable Energy: Solar Fuels Gordon Research Conference - Ventura Beach Marriott, Ventura, CA, USA.
21. **Jan 24, 2018:** Quantum Cafe Seminar on Photosynthesis - Center for Computational Quantum Physics (CCQ) of the Simons Foundation's Flatiron Institute - New York, New York, USA.
22. **Jan 13-Jan 15, 2018: Nature Conference: Materials Electrochemistry: Fundamentals and Applications - Southern University of Science and Technology, Shenzhen, China. Dec 8, 2017:** Bunty Plot Meeting - Imperial College London, London, UK.
23. **Nov 30-Dec 1, 2017:** Phi Beta Kappa Visiting Scholar Visit - University of Rochester, Rochester, NY, USA.
24. **Nov 20-21, 2017:** Workshop on Modern Developments in Quantum Chemistry - Center for Computational Quantum Physics (CCQ) of the Simons Foundation's Flatiron Institute - New York, New York, USA.
25. **Nov 13-15, 2017:** DOE Photosynthetic Systems Research PI Meeting - Gaithersburg, MD, USA.
26. **Nov 7-9, 2017:** ACS Southeast Regional Meeting - SERMACS 2017 - Charlotte, NC, USA.
27. **Nov 2-3, 2017:** Phi Beta Kappa Visiting Scholar Visit - Fairfield University, Fairfield, CT, USA.
28. **Oct 27, 2017:** Chemistry and Space Forum, University of New Haven, West Haven, CT, USA.
29. **Oct 18, 2017:** Yale 5th Annual Biophysics & Structural Biology Symposium - West Campus, Yale, New Haven, CT, USA.
30. **Oct 12-13, 2017:** Phi Beta Kappa Visiting Scholar Visit - SUNY Albany, Albany, USA.
31. **July 23, 2017:** Department of Chemistry, University of Buenos Aires - Buenos Aires, Argentina.
32. **July 16-21, 2017:** American Conference on Theoretical Chemistry - ACTC 2017 - Boston, MA, USA.
33. **June 27-29, 2017:** ACS GLRM Symposium "Photophysics and Photochemistry at Interfaces", Fargo, ND, USA.
34. **June 19-20, 2017:** ANSER Principal Investigators Workshop - Northwestern University, Evanston, IL, USA.
35. **June 11-16, 2017:** 9th International Conference on Advanced Vibrational Spectroscopy - Victoria, BC, Canada.
36. **June 5-8, 2017:** 39th DOE Solar Photochemistry Principal Investigators Meeting, Gaithersburg, Maryland.
37. **May 28-June 1, 2017:** Symposium on "Quantum Dynamical Phenomena in Chemistry" at the 100th National Meeting of the Canadian Society for Chemistry - Toronto, ON, Canada.
38. **May 23-25, 2017:** 2017 AFOSR Molecular Dynamics/Theoretical Chemistry Program Review, Philips Technology Institute (PTi) on Kirtland Air Force Base, Albuquerque, NM.
39. **May 22, 2017:** Green Photonics Using Nanostructured Semiconductors Workshop, University of Michigan, Ann Arbor, MI.

40. **May 11, 2017:** Laboratory of Computational Biology, National Heart, Lung and Blood Institute, National Institutes of Health, Bethesda, MD.
41. **May 8-11, 2017:** DOE Catalysis Scoping Meeting, Leesburg, VA.
42. **April 27-28, 2017:** 10th Annual ANSER Meeting, Northwestern University, Evanston, IL.
43. **April 2-6, 2017:** 253rd ACS National Meeting, San Francisco, CA.
44. **Feb 16-17, 2017:** 2017 Winter NIH Macromolecular Structure and Function (MFSA) Meeting, San Francisco, CA.
45. **Feb 2-3, 2017:** Arizona State University Biodesign Institute, Tempe, AZ.
46. **Jan 22-27, 2017:** 2017 Metals in Biology Gordon Research Conference (Ventura, CA).
47. **Jan 9, 2017:** DOE Catalysis Scoping Meeting, Leesburg, VA.
48. **Nov 18, 2016:** Department of Chemistry, Stony Brook University.
49. **Oct 20-21, 2016:** Annual Meeting "Energy Storage: Fundamental to Applied" - SERC 2016 - The Solar Energy Research Center of University of North Carolina at Chapel Hill, NC, USA.
50. **Oct 5, 2016:** Department of Chemistry, University of Illinois at Urbana-Champaign, IL, USA.
51. **Sept 19, 2016:** Department of Chemistry and Biochemistry, University of Arkansas, Fayetteville, AR, USA.
52. **Aug 28-Sept 2, 2016:** Conference "Theory and Applications of Computational Chemistry" - TACC 2016 - University of Washington in Seattle, WA, USA.
53. **Aug 21-25, 2016:** 252nd ACS National Meeting, Philadelphia, PA.
54. **July 17-22, 2016:** 2016 Vibrational Spectroscopy Gordon Research Conference, University of New England (Biddeford, Maine).
55. **June 21-25, 2016:** Summer School on Fundamental Science Alternative Energy, Telluride Science Research Center, Telluride, CO.
56. **June 13-17, 2016:** Excited State Processes in Electronic and Bio Nanomaterials (ESP 2016), Sante Fe, New Mexico.
57. **June 5-8, 2016:** DOE Solar Contractors Meeting, Gaithersburg, Maryland.
58. **May 24-26, 2016:** AFOSR Molecular Dynamics and Theoretical Chemistry Program Review, Arlington, Virginia.
59. **May 13-16, 2016:** KI-Net Conference on Mathematical and Computational Methods in Quantum Chemistry, Yale University. -- Photos.
60. **Apr 29-30, 2016:** Baker Symposium, Department of Chemistry, Cornell University, Ithaca, NY.
61. **Apr 27, 2016:** Department of Chemistry, Rice University.
62. **Apr 22, 2016:** Department of Chemistry, University of Colorado, Denver.
63. **March 13-17, 2016:** 251st ACS National Meeting, San Diego, CA.
64. **Feb 25-28, 2016:** Fusion Conference, Molecules and Materials for Artificial Photosynthesis, Cancun, Mexico.
65. **Jan 26-29, 2016:** Exploiting New Advances in Mathematics to Improve Calculations in Quantum Molecular Dynamics Workshop, Banff International Research Station for Mathematical Innovation and Discovery, Alberta, Canada.
66. **Jan 25, 2016:** MURI Annual Review Meeting, Chemical Reduction of Carbon Dioxide to Energy-Dense Liquids, UC-San Diego, CA.

67. **Dec 15-20, 2015:** Pacifichem 2015, Honolulu, Hawaii,USA
68. **Nov. 13-14, 2015:** 23rd International Conference on Current Trends in Computational Chemistry, Jackson, Mississippi.
69. **Oct 23, 2015:** Department of Chemistry, University of Buffalo.
70. **Oct 19-21, 2015:** NIH Panel, Washington, DC.
71. **August 16-20, 2015:** 250th ACS National Meeting, Boston, MA.
72. **August 6-9, 2015:** 2015 Beckman Symposium, Arnold and Mabel Beckman Center of the National Academies of Sciences and Engineering in Irvine, California.
73. **July 20-24, 2015:** TSRC, Quantum Effects in Condensed Phase Systems, Telluride, CO.
74. **March 22-26, 2015:** 249th ACS National Meeting, Denver, CO.
75. **Feb 19-20, 2015:** MURI Annual Review Meeting, Chemical Reduction of Carbon Dioxide to Energy-Dense Liquids, UC-San Diego, CA.
76. **Dec 14, 2014:** Workshop on Light-Driven Processes in Bio-Inspired Materials. BioScience Research Collaborative, Rice University.
77. **Dec 1, 2014:** Department of Chemistry, University of Puerto Rico, San Juan, Puerto Rico.
78. **Oct 6, 2014:** Department of Chemistry, University of Sciences, Philadephia, PA.
79. **Oct 1, 2014:** Department of Chemistry, University of Washington, Seattle
80. **Sept 30, 2014:** Department of Chemistry, University of California, Berkeley.
81. **Sept 8-12, 2014:** 16h International Congress of Photobiology, Universidad de Cordoba, Cordoba, Argentina.
82. **Sept 7, 2014:** Energizing photochemistry: Workshop satellite of the 16h International Congress of Photobiology, Universidad de Cordoba, Cordoba, Argentina.
83. **Aug 3-8, 2014:** GRC Vibrational Spectroscopy, University of New England, Biddeford, ME.
84. **Jul 13-18, 2014:** GRC Atomic and Molecular Interactions, Stonehill College, Easton, MA.
85. **June 24-28, 2014:** TSRC Summer School on Alternative Energy, Telluride, CO.
86. **April 15, 2014:** University of Zurich, Switzerland.
87. **March 16-20, 2014:** 247th ACS National Meeting, Dallas, Texas.
88. **Feb 6-9, 2014:** Molecules and Materials for Artificial Photosynthesis Conference,Cancun, Mexico.
89. **Dec 9, 2013:** MURI Meeting, Department of Chemistry, UC San Diego.
90. **Nov 28-Dec. 1, 2013:** CECAM Workshop on Quantum Dynamics in Molecular and Nano-Materials: Mechanisms and Functionality, Tel Aviv University, Israel.
91. **Nov 7, 2013:** Department of Chemistry, Northwestern University.
92. **Oct 15, 2013:** Department of Chemistry, Wayne State University.
93. **Oct 3, 2013:** NIH Study Section, Washington DC.
94. **Sept 30, 2013:** Department of Chemistry, University of South Dakota.
95. **Sept 8-12, 2013:** Physical Chemistry of Solar Energy Conversion Symposium, 246th (Fall 2013) ACS National Meeting, Indianapolis, Indiana.
96. **Aug 16-20, 2013:** Summer School on Mathematical and Computational Methods in Quantum Dynamics at the University of Wisconsin-Madison.